

# A Configurationally-Resolved-Super-Transition-Arrays method for calculation of the spectral absorption coefficient in hot plasmas.

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(Dated: March 2, 2013)

## Abstract

A new method, 'Configurationally-Resolved-Super-Transition-Arrays', for calculation of the spectral absorption coefficient in hot plasmas is presented. In the new method, the spectrum of each Super-Transition-Array is evaluated as the Fourier transform of a single Complex Pseudo Partition Function, which represents the *exact* analytical sum of the contributions of all constituting unresolved transition arrays sharing the same set of one-electron solutions. Thus, in the new method, the spectrum of each Super-Transition-Array is resolved down to the level of the (unresolved) transition arrays. It is shown that the corresponding spectrum, evaluated by the traditional Super-Transition-Arrays (STA) method [A. Bar Shalom, J. Oreg, W.H. Goldstein, D. Shvarts and A. Zigler, Phys. Rev. A **40**, 3183 (1989)], is just the coarse grained Gaussian approximation of the Configurationally-Resolved-Super-Transition-Array. A new computer program is presented, capable of evaluating the absorption coefficient by both the new configurationally resolved and the traditional Gaussian Super-Transition-Arrays methods. A numerical example of gold at temperature  $1keV$  and density  $0.5\text{ gr/cm}^3$ , is presented, demonstrating the simplicity, efficiency and accuracy of the new method.

## I. INTRODUCTION

The radiative opacity is an essential factor governing the structure and evolution of stars [1],[2] as well as laboratory plasmas[3]. In plasmas containing medium to high  $Z$  elements, at least some of the electrons remain bound to the ions even at very high temperatures and densities (e.g. iron at the center of the sun). As was first recognized by Edward Teller[4], in part of the spectral range, the opacity in these plasmas is dominated by photo-absorption of dipolar radiative transitions between electronic states of the ions (line absorption).

The present work focuses on line absorption in plasmas in Local Thermodynamic Equilibrium (LTE). Historically, the development of the theory and computational approach to this process required a major theoretical effort(e.g. [5], [6], [7]). The atomic states are evaluated, in all methods, by a perturbation expansion, using the radial average potential approximation as the zero order. In this order, the equation for the many-electron states is reduced to equations for the one-electron states in an average radial self-consistent potential due to all other electrons. For light elements, Schroedinger equation is sufficient, for heavier elements, relativistic treatment is required and the Dirac equation should be solved. The zero order many-electron states ("configurations") and energies are characterized by the occupation numbers of degenerate groups of one-electron states ("shells"). Mutual electron-electron interaction removes the degeneracy and splits the configurational energy. This effect is evaluated as a first order correction. i.e. as the sum of expectation values, in the zero order states, of energies due to coulomb interaction between all pairs of electrons. The well known Slater integrals represent the radial part of these expectation values.

The evaluation of the absorption coefficient requires a compromise between the needed spectral resolution and the available computer resources (for a representative list of codes see e.g. [8],[9],[10]). Existing methods may be classified according to the resolution of the description of electronic states, and of the contribution of transitions between them to the absorption coefficient. The most resolved treatment available is the Detailed Line Accounting (DLA, e.g. [11]). For complex configurations with many states, the number of transitions becomes prohibitive for numerical calculations. In this case, one may turn to the Unresolved-Transition-Arrays (UTA) method. In this method the spectral absorption coefficient due to a transition array consisting of all single-electron transitions between a specific pair of configurations is assumed to be of a Gaussian shape. This method is made practical by

the analytical formulae for the three lowest energy-moments (actually cumulants[12]) of the UTA spectrum[13], in terms of reduced matrix elements of the dipole operator, Slater integrals and shell occupation numbers. For heavy ions, the UTA method becomes unpractical due to the enormous number of possible configurations. The Super-Transition-Array (STA) method[14],[15],[16] represents a further compromise which allows the evaluation of opacity with less computational effort at the cost of spectral coarse graining. The coarse graining is obtained by grouping shells, with adjacent energies, into supershells, configurations into superconfigurations (SCs) and correspondingly transition arrays into supertransition arrays. The relative simplicity of the evaluation of the coarse-grained spectral absorption coefficient is based on three assumptions (on top of the UTA assumption):

a) *The basic superconfiguration assumption:* All configurations which form a superconfiguration share the same radial potential with the same set of one-particle solutions.

b) *The high-temperature approximation:* The spread of the energies of configurations within a superconfiguration is much smaller than the plasma temperature. In this limit the Boltzmann factor which determines the relative probability for a configuration within a superconfiguration may be evaluated to zero order only, i.e. as the sum of single-electron energies in the mean potential. Electron-electron interaction energy adds a superconfigurational average factor common to all configurations within a superconfiguration. This corresponds to the use of the Gibbs-Bogoliubov-Feynman bound [17] as an estimate for the Boltzmann factor.

c) *The unresolved supertransition array assumption:* The spectra of all UTAs which form a STA merge into a single Gaussian shape.

With these three approximations the summation of contributions of all UTAs to a STA may be performed analytically [14],[15]. By the third approximation, one needs only to evaluate the three lowest energy cumulants of the STA spectrum. By the second approximation, the relative probabilities of configurations are the same as of those in a system of independent particles in a potential well [18]. This enables the derivation of analytical formulae for the moments (and cumulants) in terms of Slater integrals and partition functions[14],[16] which may be evaluated by recursion relations [14],[20],[21].

In reference [23], a way to avoid the high-temperature approximation was shown. An analytical formula was written for the partition function with the full Hamiltonian including electron-electron interaction. This result was enabled by the application of the Hubbard-

Stratonovich transformation [24], which eliminates of the quadratic dependence of the energy on the shell occupation numbers (at the cost of introduction of an auxiliary random field).

The approximations in assumptions (a)-(c) are controlled by the choice of the degree of spectral coarse graining. In the extreme choice of one shell in a supershell, and one configuration in a superconfiguration, and a different average radial potential with a different set of one-electron states separately for each configuration, one reaches the UTA limit. Clearly, within the framework of the UTA model, assumptions (a)-(c) are exactly satisfied. The opposite extreme choice is of one supershell consisting of all shells and one superconfiguration consisting of all configurations in all degrees of ionization. In reference [14] it was shown that this choice of maximum spectral coarse graining reproduces the results of the average atom (AA) model, presented in reference [25].

As mentioned above, for heavy ions, calculations with the UTA resolution are impractical due to the enormous number of possible configurations. On the other hand, the AA model is too crude since it wipes out the spectral structure observed in experiments [14]. The STA method allows for a tune up of the resolution by an iterative refinement procedure starting from the AA model, increasing the number of superconfigurations and number of different radial potentials with different sets of one-particle solutions. The refinement process is stopped when both the values Rosseland and Planck mean free path (MFP)[1] converge to constant values. A typical STA run reaches convergence with a few to a few tens of SCF solutions per degree of ionization, and many more superconfigurations sharing the same potential and set of single particle energies and orbitals. Actually, as will be demonstrated by the numerical example in the present work, when a strict convergence test based on the spectral details rather than the integrated values of Rosseland and Planck MFP is imposed, convergence of the STA refinement process in heavy elements is not fully reached even with half a million STAs.

In the present work, we derive a formula for the spectrum of Configurationally-Resolved-Super-Transition-Arrays (CRSTA) which represents the *exact sum* of the spectra of all UTAs constituting the STA and sharing the same SCF solution. Out of the three assumptions ((a)-(c) mentioned above), required by the traditional STA method, only the basic superconfiguration assumption (a) was used in the derivation of our new CRSTA method. As a consistency check we show that the radiation intensity, average energy and variance of the standard STAs are recovered from the CRSTA by an approximation based on a cu-

mulant expansion, truncated at the third term. i.e., the spectrum of a STA evaluated by the traditional method is the coarse-grained Gaussian approximation of the spectrum of the corresponding CRSTA.

The plan of the manuscript is as follows: In section II, some well known formulae required for the evaluation of the absorption coefficient in terms of the two-time dipole autocorrelation function[26],[12],[27],[28] expanded in the eigenstates of the atomic Hamiltonian are summarized. The STA order of summation is briefly reviewed in section III. In section IV the formula for the CRSTA spectrum is derived. This formula is limited to the simple case where the Boltzmann factor is evaluated only with zero-order energies and the widths of the UTA are neglected (as in the original STA paper[14]). The derivation of the formula for the general case with the effect of electron-electron interaction in the Boltzmann factor and with the inclusion of the width of the UTA is derived in the Appendix. Section V contains a brief description of our new code, for the evaluation of the spectral absorption coefficient by both the standard STA and the new CRSTA methods, and a numerical example demonstrating the simplicity efficiency and accuracy of the new CRSTA method. A Summary and discussion are presented in section VI.

## II. THE ABSORPTION COEFFICIENT

The absorption coefficient, in hot dense plasmas in LTE, may be written in terms of the two-time autocorrelation function of the atomic many-electron dipole [12],[26],[27],[28],[29]:

$$\mu_{\text{at}}(E) = E^2 \frac{4\pi}{3} \frac{e^2}{\hbar c} n_0 \text{Re} \left\{ \int_0^\infty C_K(\tau) e^{iE\tau/\hbar} d\tau \right\}. \quad (1)$$

$\mu_{\text{at}}$  is defined as the fraction of the net absorbed radiation energy at energy  $E$  per unit radiation propagation length.  $n_0$  is the atoms number density,  $C_K(\tau)$  is the two-time autocorrelation function of the atomic many-electron dipole[26]:

$$C_K(\tau) = \beta \text{trace} \left( \rho_{\text{eq}} d(\tau) \tilde{d}(\beta) \right). \quad (2)$$

Eq. (1) is just one of many manifestations of the fluctuation-dissipation theorem connecting between the response of a given system to an external disturbance and the correlation of internal fluctuations of the system in the absence of the disturbance [29]. In Eq. (2),  $\rho_{\text{eq}}$

is the equilibrium density matrix;  $d(\tau)$  is the the projection of the Heisenberg representation of the atomic dipole operator,  $\sum_i \vec{r}_i$ , on the polarization vector of the radiation field, (averaging over all possible polarizations is implied).  $\vec{r}_i$  is the position operator of the  $i$ 'th electron.  $\tilde{d}$  denotes the Kubo transform of  $d$ :

$$\tilde{d}(\beta) = \frac{1}{\beta} \int_0^\beta d(i\hbar\lambda) d\lambda. \quad (3)$$

(For the relation between the correlation function  $C_K$  and more commonly used functions such as the symmetrized correlation function  $C(\tau) = \frac{1}{i\hbar} \text{trace}(\rho_{\text{eq}}(d(\tau)d(0) + d(0)d(\tau)))$ , see references [26],[12],[27]).

Expanding the dipole and the density operators in eigenfunctions of the atomic Hamiltonian,  $H$ , with energies  $\{E_n\}$  using:

$$(\rho_{\text{eq}})_{nn} = \frac{e^{-\beta(E_n - Q\mu)}}{\sum_n e^{-\beta(E_n - Q\mu)}}, \quad (4)$$

where  $Q$  is the number of electrons,  $\mu$  is the chemical potential,  $\beta = 1/k_B T$ ,  $T$  is the temperature and  $k_B$  is the Boltzmann constant, the formula for  $\mu_{\text{at}}$  becomes:

$$\mu_{\text{at}}(E) = E^2 \frac{4\pi}{3} \frac{e^2}{\hbar c} n_0 \frac{1 - e^{-\beta E}}{E} \text{Re} \int_0^\infty \vartheta(\tau, \beta) e^{-iE\tau/\hbar} d\tau, \quad (5)$$

with

$$\vartheta(\tau, \beta) = \frac{1}{\sum_i e^{-\beta(E_i - Q\mu)}} \sum_{i,f} e^{-\beta(E_i - Q\mu)} |d_{if}|^2 e^{-i(E_i - E_f)\tau/\hbar} \quad (6)$$

and  $\vec{d}_{if} = \langle i | \vec{d} | f \rangle$ . Eq. (5) is equivalent to the Fermi golden rule in the form used in [14][15]. This can be easily seen by performing the  $\tau$  integral and using the relation  $\delta(E_f - E_i - E) = \frac{1}{\pi} \lim_{\gamma \rightarrow 0} \text{Im} \left\{ \frac{1}{E_f - E_i - E - i\gamma} \right\}$ . However, as will become clear from the results below, the summation over states becomes an easier task when performed prior to the  $\tau$  integration.

### III. SUMMATION OVER CONFIGURATIONS

Eq. (6) is a formula for  $\vartheta$  in terms of the exact many-electron energies and dipole matrix elements. As described in the introduction, in practice, these quantities are evaluated by a perturbation expansion, using the radial average potential approximation as the zero order. A configuration is a zero order many-electron state described by the occupation numbers

of the shells. Symbolically, a configuration is written as  $C = \prod_s (n_s l_s j_s)^{q_s}$  where a shell is defined by the principal quantum number  $n_s$ , the orbital angular momentum of the large component in the Dirac wave function,  $l_s$ , and the total orbital+spin angular momentum  $j_s$ ;  $q_s$  is the occupation number of the shell (configurations are degenerate states). Mutual electron-electron interaction lifts the degeneracy and splits the configurational energy. This effect is evaluated as a first order correction, i.e. as the sum of expectation values, in the zero order states of energies due to coulomb interaction between all pairs of electrons. In principle, to evaluate the first-order correction one should diagonalize the perturbation within each degenerate subspace. The methods discussed here involve only configurational averaged quantities, i.e. taking the trace, a process which does not require the diagonalization.

Based on this picture, the STA method [14][15] splits the summation in Eq. (6) into a few stages. First, the spectrum is split into the different contributions of one-electron transitions, i.e.:

$$\vartheta = \sum_{a,b} \vartheta^{ab}, \quad (7)$$

where  $\vartheta^{ab}$  is the spectrum due to all possible transitions in which an electron transits from the shell  $n_a l_a j_a$  to another shell  $n_b l_b j_b$ . The summation is over all configurations  $C$  in which the shell  $a$  has at least one electron i.e. the occupation number is  $q_a > 0$  and the shell  $b$  has at least one hole, i.e.  $q_b < 2j_b + 1$ . The summation over all accessible configurations is further partitioned by introducing an intermediate summation step over superconfigurations  $\Xi$ [14][15]:

$$\vartheta^{ab} = \frac{1}{N} \sum_{\Xi} \left( \sum_{C \in \Xi} g_C \exp(-\beta(E_C - Q\mu)) \right) \sum_{C \in \Xi} \frac{g_C \exp(-\beta(E_C - Q\mu))}{\sum_{C \in \Xi} g_C \exp(-\beta(E_C - Q\mu))} \vartheta_C^{ab}, \quad (8)$$

where  $N = \sum_{\Xi} \sum_{C \in \Xi} g_C \exp(-\beta(E_C - Q\mu)) = \sum_{\text{All } C} g_C \exp(-\beta(E_C - Q\mu))$ .

Each superconfiguration represents a particular distribution of the electrons between supershells (a group of energetically adjacent atomic shells).

In Eq.(8),  $\vartheta_C^{ab}$  represents the contributions from the transition array  $C^{ab}$ , composed of all transitions from the shell  $n_a l_a j_a$  in the configuration  $C$  to the shell  $n_b l_b j_b$ , and  $g_C$  is the zeroth order degeneracy. Following the STA method, we adopt the assumption of the UTA approach [13], that these transitions merge into an unresolved spectrum of a Gaussian shape

(i.e a UTA). Thus, the three lowest energy moments of the UTA  $f_C^{ab} E_C^{ab} (\Delta E_C^{ab})^2$  are used to construct the spectrum. In the context of the present work this means

$$\vartheta_C^{ab}(\tau, \beta) = f_C^{ab} \exp \left\{ -\frac{1}{2} (\Delta E_C^{ab})^2 \tau^2 + i E_C^{ab} \tau \right\} \quad (9)$$

and:

$$\begin{aligned} \vartheta_{\Xi}^{ab} &\equiv \frac{1}{\sum_{C \in \Xi} g_C e^{-\beta(E_C - Q\mu)}} \sum_{C \in \Xi} g_C \exp(-\beta(E_C - Q\mu)) \vartheta_C^{ab}(\tau, \beta) \\ &= \frac{1}{\sum_{C \in \Xi} g_C e^{-\beta(E_C - Q\mu)}} \sum_{C \in \Xi} f_C^{ab} g_C \exp \left\{ \Phi_C^{ab}(\{q^C\}, \beta, \tau^2, i\tau) \right\}, \end{aligned} \quad (10)$$

where

$$\Phi_C^{ab}(\{q^C\}, \beta, \tau^2, i\tau) \equiv -\beta(E_C - Q\mu) - \frac{1}{2} (\Delta E_C^{ab})^2 \tau^2 + i E_C^{ab} \tau. \quad (11)$$

The moments of the UTA are represented in the following compact formulae [14]; The strength of a transition is:

$$f_C^{ab} = q_a^C (g_b - q_b^C) (\langle a || r || b \rangle)^2, \quad (12)$$

where  $\langle a || r || b \rangle$  is the reduced matrix element of the dipole. The configurational average of the energy is:

$$E_C = \sum_s q_s \langle s \rangle + \frac{1}{2} \sum_s \sum_r q_s (q_r - \delta_{rs}) \langle s, r \rangle, \quad (13)$$

with

$$\langle s \rangle \equiv \varepsilon_s + \left\langle s \left| -V(r) - \frac{Z}{r} \right| s \right\rangle \quad (14)$$

and

$$\langle s, r \rangle = F^0(s, r) - \frac{1}{2} \frac{g_s}{g_s - \delta_{s,r}} \sum_k (1 - \delta_{sr} \delta_{k0}) \begin{pmatrix} j_s & k & j_r \\ 1/2 & 0 & -1/2 \end{pmatrix}^2 G^{(k)}(s, r), \quad (15)$$

where  $F^{(k)}, G^{(k)}$  are the Slater integrals corresponding to direct and exchange interaction,  $\begin{pmatrix} j_s & k & j_r \\ 1/2 & 0 & -1/2 \end{pmatrix}$  is the  $3j$  Symbol, and  $l_s, k, l_r$  obey the triangle inequality.

The center of gravity of the UTA is:

$$E_C^{ab} = D_0^{ab} + \sum_s (q_s - \delta_{sa}) \left( D_s^{ab} + \left( \frac{\delta_{sa}}{g_s - 1} - \frac{\delta_{sb}}{g_s - 1} \right) \varphi(a, b) \right), \quad (16)$$



where:

$$D_0^{ab} = \langle b \rangle - \langle a \rangle, \quad (17)$$

$$D_s^{ab} = (\langle s, b \rangle - \langle s, a \rangle) \quad (18)$$

and

$$\begin{aligned} \varphi(a, b) \equiv & - \sum_{\substack{k \neq 0 \\ \text{even}}} g_a g_b \left\{ \begin{matrix} k & j_a & j_a \\ 1 & j_b & j_b \end{matrix} \right\} \left( \begin{matrix} j_a & k & j_a \\ \frac{1}{2} & 0 & -\frac{1}{2} \end{matrix} \right)^2 \left( \begin{matrix} j_b & k & j_b \\ \frac{1}{2} & 0 & -\frac{1}{2} \end{matrix} \right)^2 F^{(k)}(a, b) \\ & + \sum_k \frac{g_a g_b \delta_{k,1-3}}{3} \left( \begin{matrix} j_a & k & j_b \\ \frac{1}{2} & 0 & -\frac{1}{2} \end{matrix} \right)^2 \frac{1+(-1)^{l_a+l_b+k}}{2} G^{(k)}(a, b). \end{aligned} \quad (19)$$

The variance of the UTA is:

$$(\Delta E_C^{ab})^2 = \sum_s (q_s - \delta_{sa}) (q_s - q_s - \delta_{sb}) (\Delta^2)_s^{ab}, \quad (20)$$

where  $(\Delta^2)_s^{ab}$  is independent of the occupation numbers.

These are all the building blocks necessary for the summation in Eq. (10).

#### IV. CONFIGURATIONALLY-RESOLVED-SUPER-TRANSITION-ARRAYS

For the simplicity of presentation we focus on the case in which the width of the UTA,  $(\Delta E_C^{ab})^2$ , as well as the electron-electron interaction terms in the Boltzmann factor, i.e. in  $E_C$  (but not in  $E_C^{ab}$ ), are ignored. The treatment of the general case is deferred to the Appendix. Ignoring the width of the UTA, as well as the electron-electron interaction terms in  $E_C$ , Eq.(10) is reduced to:

$$\vartheta_{\Xi}^{ab} = \frac{1}{\sum_{C \in \Xi} g_C e^{-\beta(E_C - Q\mu)}} \sum_{C \in \Xi} g_C e^{-\beta(E_C - Q\mu)} f_C^{ab} e^{iE_C^{ab}\tau/\hbar}, \quad (21)$$

where the zeroth order degeneracy is:  $g_C = \prod_{s \in C} \binom{g_s}{q_s^C}$ . The Fourier transform yields the STA spectrum. The standard STA method [14] may be obtained by a cumulant expansion ([12]) of Eq. (21) and truncation at the third cumulant. This may be seen by writing the Taylor series for the factor  $e^{iE_C^{ab}\tau/\hbar}$ , to obtain the expansion:

$$\vartheta_{\Xi}^{ab} = \frac{1}{U_{\Xi}} f_{\Xi}^{ab} \sum_{n=0}^{\infty} \frac{1}{n!} (i\tau/\hbar)^n \mu_n^{\Xi ab}, \quad (22)$$

where:

$$\mu_n^{\Xi ab} = \frac{1}{f_{\Xi}^{ab}} \sum_{C \in \Xi} g_C e^{-\beta(E_C - Q\mu)} f_C^{ab} (E_C^{ab})^n \quad (23)$$

and  $f_{\Xi}^{ab} = \sum_{C \in \Xi} g_C e^{-\beta(E_C - Q\mu)} f_C^{ab} = \mu_0^{\Xi ab}$ .

Using the Gaussianity assumption,

$$\begin{aligned} \vartheta_{\Xi}^{ab}(\tau, \beta) &= I_{\Xi}^{ab} \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi(\Delta\varepsilon_{\Xi}^{ab})^2}} \exp\left[-\frac{1}{2} \frac{(E - \varepsilon_{\Xi}^{ab})^2}{(\Delta\varepsilon_{\Xi}^{ab})^2}\right] e^{iE\tau/\hbar} dE \\ &= I_{\Xi}^{ab} e^{-i\varepsilon_{\Xi}^{ab}\tau - \frac{1}{2}(\Delta\varepsilon_{\Xi}^{ab})^2\tau^2} \end{aligned} \quad (24)$$

yields the total radiation intensity, average energy and variance of the STA. Explicitly,

$$I_{\Xi}^{ab} = [\vartheta_{\Xi}^{ab}(\tau, \beta)]_{\tau=0} = \frac{1}{U_{\Xi}} f_{\Xi}^{ab}, \quad (25)$$

$$\varepsilon_{\Xi}^{ab} = \left[ \frac{\partial}{\partial(-i\tau/\hbar)} \ln \left( \frac{\vartheta_{\Xi}^{ab}(\tau, \beta)}{I_{\Xi}^{ab}} \right) \right]_{\tau=0} = \frac{\mu_1^{\Xi ab}}{\mu_0^{\Xi ab}}, \quad (26)$$

$$(\Delta\varepsilon_{\Xi}^{ab})^2 = \left[ \frac{\partial^2}{\partial(-i\tau/\hbar)^2} \ln \left( \frac{\vartheta_{\Xi}^{ab}(\tau, \beta)}{I_{\Xi}^{ab}} \right) \right]_{\tau=0} = \frac{\mu_2^{\Xi ab}}{\mu_0^{\Xi ab}} - \left( \frac{\mu_1^{\Xi ab}}{\mu_0^{\Xi ab}} \right)^2. \quad (27)$$

These results coincide with Eqs. (20),(21),(22) in reference [14]. In the practical application of the standard STA method, one is enforced to represent the spectrum by a large number of narrow Gaussian STAs, in order to minimize the error due to the truncation of the series. Typically, a STA run uses only a few self-consistent potentials (and sets of one-particle states and energies) for every degree of ionization, but a multitude of STAs. Thus, a multitude of STAs (and many more UTAs) share the same set of one-particle states and energies.

Our new CRSTA method avoids the approximation of Gaussian STAs (i.e. the approximation in the truncation at the second cumulant). This is done by the application of the mathematical machinery of partition functions of independent particles directly to the contribution of transition arrays (actually their Fourier transform), to obtain the exact sum of all UTAs sharing the same one-particle states and energies. Explicitly, this is done by absorbing the time dependent exponent in the Boltzmann factor and using Eqs.(13), (16) to write the exponential factors in Eq. (21) as:

$$\begin{aligned} &g_C e^{-\beta(E_C - Q\mu)} e^{iE_C^{ab}\tau/\hbar} \\ &= e^{-i(D_0^{ab} - D_a^{ab})\tau/\hbar} \prod_{s \in C} \left( \frac{g_s}{q_s^C} \right) e^{-q_s^C \{ \beta(\varepsilon_s - \mu) + iD_a^{ab}\tau/\hbar \}} \\ &= e^{-i(D_0^{ab} - D_{\alpha}^{ab})\tau/\hbar} \prod_{s \in C} \left( \frac{g_s}{q_s^C} \right) (X_s^{ab}(\beta, \tau))^{q_s^C}, \end{aligned} \quad (28)$$

where:

$$X_s^{ab}(\beta, \tau) = e^{-\{\beta(\varepsilon_s - \mu) + iD_s^{ab}\tau/\hbar\}}. \quad (29)$$

Next, we define the "superconfigurational degeneracy vector" with components  $(\vec{g})_s = g_s$  and the supertransitional "Complex Pseudo Partition Function" (CPPF):

$$U_{\Xi}^{ab}(\vec{g}, \beta, \tau) = \sum_{C \in \Xi} \prod_{s \in C} \binom{g_s}{q_s^C} (X_s^{ab}(\beta, \tau))^{q_s^C} \quad (30)$$

and

$$U^{ab}(\vec{g}, \beta, \tau) = \sum_{\Xi} U_{\Xi}^{ab}(\vec{g}, \beta, \tau). \quad (31)$$

Using the well known combinatorial relations  $q \binom{g}{q} = g \binom{g-1}{q-1}$  and  $(g-q) \binom{g}{q} = g \binom{g-1}{q}$ , one gets:

$$\begin{aligned} \vartheta_{\Xi}^{ab} &= \frac{(\langle a||r||b \rangle)^2 e^{-i(D_0^{ab} - D_a^{ab})\tau/\hbar}}{U_{\Xi}^{ab}|_{\tau=0}} \sum_{C \in \Xi} \prod_{s \in C} \binom{g_s}{q_s^C} (X_s^{ab})^{q_s^C} q_a^C (g_b - q_b^C) \\ &= \frac{(\langle a||r||b \rangle)^2 e^{-i(D_0^{ab} - D_a^{ab})\tau/\hbar}}{U_{\Xi}^{ab}|_{\tau=0}} g_a g_b X_a^{ab} \sum_{C \in \Xi} \prod_{s \in C} \binom{g_s - \delta_{sa} - \delta_{sb}}{q_s^C - \delta_{sa}} (X_s^{ab})^{q_s^C - \delta_{sa}} \\ &= \frac{(\langle a||r||b \rangle)^2 e^{-i(D_0^{ab} - D_a^{ab})\tau/\hbar}}{U_{\Xi}^{ab}|_{\tau=0}} g_a g_b X_a^{ab} U_{\Xi, Q-1}^{ab}(\vec{g} - \vec{\delta}_a - \vec{\delta}_b, \beta, \tau). \end{aligned} \quad (32)$$

In Eq.(32), the length of the vector  $\vec{\delta}_a$  equals to the number of shells, where all components vanish except for the  $a$  component which has the value of 1.

Note that the algebraic dependence of the formula for the partition function, Eq. (30), on the degeneracies, shell occupation numbers and  $X$  is the same as of the standard partition function. Therefore, it obeys the same recursion relations and is accessible to the efficient evaluation methods [14][15],[19],[20],[21]. Unlike references [14][15],[19],[20],[21] where the partition function is used for the evaluation of the energy-moments of the spectrum, Eqs. (32) when Fourier Transformed with respect to time expresses the STA spectrum itself as a partition function.

Finally, the formula for the spectral absorption coefficient is obtained by using Eqs. (32) and (5):

$$\begin{aligned} \mu_{\text{at}}(E) = & \frac{4\pi}{3} \frac{e^2}{\hbar c} \frac{E}{\hbar} n_0 (1 - e^{-\beta E}) \frac{1}{U|_{\tau=0}} \sum_{\Xi, a, b} (\langle a || r || b \rangle)^2 g_a g_b \\ & \times \text{Re} \int_0^\infty e^{-i(D_0^{ab} - D_a^{ab})\tau/\hbar} X_a^{ab} U_{\Xi, Q-1}^{ab} \left( \vec{g} - \vec{\delta}_a - \vec{\delta}_b, \beta, \tau \right) e^{-iE\tau/\hbar} d\tau. \end{aligned} \quad (33)$$

## V. NUMERICAL EXAMPLE

We have written, from scratch, a new numerical code called CRSTA. This code can calculate the spectral absorption by two optional methods, the standard STA[14],[30] method and our new CRSTA method. In the STA method, single-particle energies are used to construct the real partition functions, which in turn are used together with the Slater integrals to construct the total intensity, average energy and variance of the STA. The spectrum of each STA is constructed as a Voigt function, which accounts for STA width as well as Doppler and electron impact effects. The absorption spectrum is obtained by the summation of contributions from all STA's. In the CRSTA method, single-particle energies and Slater integrals are used to construct the CPPF at different times (Eq. (30)), from which the spectral absorption coefficient is evaluated by Eq.(33).

The focus of the the illustrating example was on the replacement of the traditional STA method of summation over configurations, which is based on the Gaussian approximation, by the CRSTA method in which the summation is exact (within the framework of the basic superconfiguration assumption (a)). Naturally, important technical and physical issues, which are common to the traditional and the new methods (such as stable and effecient evaluation of the partition function, and modeling of plasma effects ([19]),([30])), where out of the focus of the present work. These issues where treated, in the present work, by the simplest possible methods.

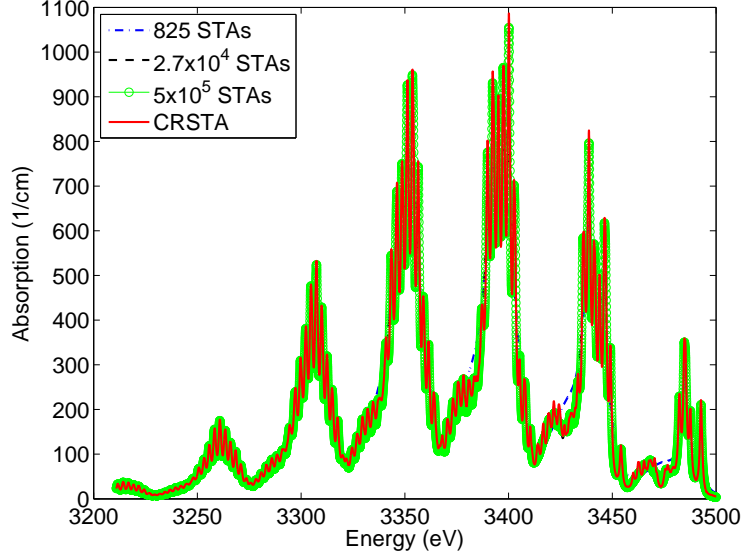
In both the new and traditinal methods, the relativistic single-particle radial eigenfunctions and eigenvalues are obtained from a self consistent solution (SCF) of the radial Dirac equation with the Hartree-Fock-Slater (HFS) potential in an ion-sphere. In our illustrating example, we use a SCF procedure, based on a very simple plasma model, that is briefly decribed as follow. In the first stage, an AA SCF calculation is done, providing the chemical potential and the average ionized electrons number. The chemical potential enforces neutrality within the AA's ion-sphere cell, where the free electrons density is approximated

by Thomas-Fermi model. In the second stage, a single SCF is calculated for each Q state (containing a single supershell and superconfiguration). For simplicity, we model each Q state as an ion-sphere that contains Q electrons and embedded in a uniform free electrons density,  $\rho_0$ . The former is calculated as the AA's ionized electrons number divided by the AA's cell volume. The neutrality of each Q state's ion-sphere is obtained by choosing its radius,  $r_Q$ , as:  $Q + 4/3\rho_0\pi r_Q^3 = Z$ .

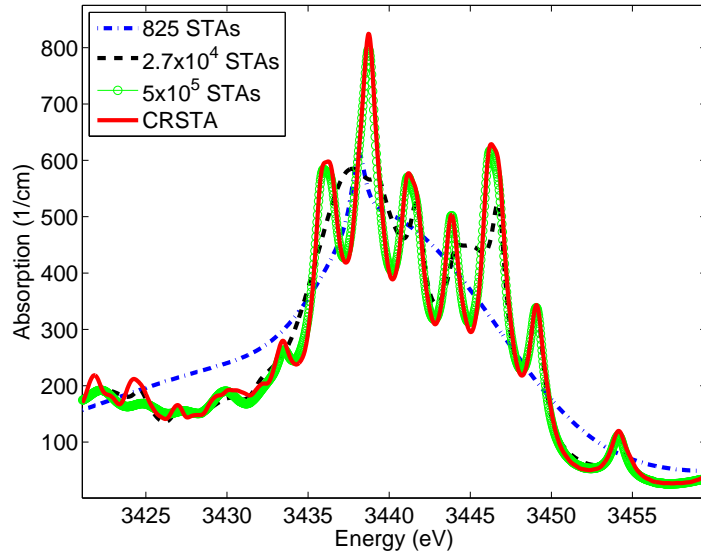
The STA method requires two refinement loops. In the external refinement loop, the number of SCs sharing one-particle solutions with the same HFS potential is decreased. For example, in the AA limit, only one potential is used for all possible configurations sharing the same potential. In reference [14] a different potential is used for each degree of ionization. Further refinement and convergence is obtained when few potentials are used for each degree of ionization. Yet, further spectral resolution is obtained by an additional internal loop, in which the number of Gaussian STAs sharing the same HFS solution is increased. In the CRSTA method, the internal loop of refinement is not necessary, since the exact analytical sum of contributions from all configurations sharing the same potential is represented by a single CPPF. On the other hand, the CRSTA method requires evaluation of CPPF on a time grid. We calculate the CPPFs using the fast recursion formulas of Bar-Shalom *et al.* [14], by substituting the complex quantity  $X_s^{ab}(\beta, \tau)$  rather than the standard  $X_s(\beta)$  ( $= X_s^{ab}(\beta, 0)$ ). Of course, the complex factor of  $X_s^{ab}(\beta, \tau)$  does not affect the numerical stability/instability of these formulas, therefore, one can use the same alternative stable methods [19]- [22], by substituting  $X_s \mapsto X_s^{ab}(\beta, \tau)$ , when numerical instabilities are expected (in our numerical example, we freeze several lowest energy shells to be fully occupied, and account small electrons number to be active in several supershells, therefore, instability is not expected). In our calculation, for each SCF potential,  $V_j$ , and allowed transition,  $a_j \rightarrow b_j$ , where  $a_j$  and  $b_j$  are bound ionic shells we define a time grid. The resolution and size of the time grid are determined from the zeroth order transition energies, and an estimation of the expected width,  $\Gamma$ . Rapid oscillations in the integrand are eliminated by utilizing the fact that the Fourier transform (FT) in Eq. (33) equals to the FT of the function  $X_a^{ab}(\tau)U_{\Xi, Q-1}^{ab}(\vec{g} - \vec{\delta}_a - \vec{\delta}_b, \beta, \tau)$ , shifted by the energy  $D_0^{ab} - D_a^{ab}$ . The time resolution,  $\Delta t$ , is estimated as  $2\pi/\Delta t = n \times |\varepsilon_\beta - \varepsilon_\alpha| \times w$ , and the time interval as  $[0, 2m/\Gamma]$ , where typically  $2 < n < 5$ ,  $m \geq 4$  and  $0.1 \leq w < 0.3$ . In order to incorporate impact broadening effects, we also multiply by the factor  $\exp(-\Gamma/2\tau)$  prior to the Fourier Transform. Typically, only

some 100-1000 CPPF calculations are required for each transition  $a_j \rightarrow b_j$ , in order to obtain a UTA like resolution of the spectrum.

Figure (1) shows the b-b absorption spectrum of the  $3p_{3/2} \rightarrow 4d_{5/2}$  transition in a Gold plasma at temperature of  $1keV$  and density of  $0.5gr/cm^3$ , (see similar example in p. 227 in Ref. [7]). Only zero order energies are used in the evaluation of the partition function and the widths of the UTAs are ignored [14] (See however reference [15] and Appendix VII). Also, for the sake of simplicity we have used a single potential for each degree of ionization, having the ionic states  $Q = 11..21$  (shells below  $3s$  shell remain fully occupied for these Q-states). The time grids contain 2000 grid points and resolution of  $0.15a.u.$  The electron impact parameter,  $\Gamma \approx 0.04a.u.$ , is calculated from the simple model of section 7.1.2 in Ref. [6]. For comparison, we have also evaluated the spectrum by the STA method with increasing number of supershells, and correspondingly increasing number of superconfigurations and Gaussian STAs. Figure (2) focuses on the energy range 3420-3460 eV. Clearly, a convergence is obtained only when a huge number of STAs (half a million) is used. Note that in the range 3420-3430 eV even half a million of STAs do not fully reveal the spectral details. In this case, half a million partition functions and half a million recursion formulas were calculated for the energy and variance of each STA. In addition, half a million Voigt profiles were calculated for each STA. On the other hand, in the CRSTA calculation, only 22,000 CPPF and 11 FTs were calculated. In order to check the analytical convergence of the STA spectrum to the CRSTA spectrum, we have also calculated an extreme case of a UTA spectrum of a low ionic state,  $Q = 14$ , where only four electrons out of the 14 remain unfrozen and play an active combinatorial role. For this check, the STA spectrum is calculated as a sum of Lorentzian profiles, rather than Gaussians. The CRSTA and STA spectral profiles in this extreme case (not shown here) completely coincide.



Figure(1): b-b absorption spectrum of gold at  $T = 1keV$  and  $\rho = 0.5 g/cm^3$



Figure(2) Zoom of the energy range 3420-3460 eV in Figure(1)

## VI. SUMMARY AND DISCUSSION

The main result of the present work is in Eqs. (32) and (36),(37) for the evaluation of the spectrum of a STA in terms of a single CPPF. In order to analyze the difference between the new CRSTA method and the traditional STA method let us examine the derivation starting from Eq. (21). This equation contains an instruction to sum over all the transitions constituting the STA,  $\Xi$ , to get the Fourier transform of the STA spectrum,  $\vartheta_{\Xi}^{ab}(\tau, \beta)$ . The traditional STA formula for  $\vartheta_{\Xi}^{ab}$  is obtained by Taylor expansion with respect to  $\tau$ , (Eq.

(22)). The Gaussian assumption (Eq. (24)), leads to the truncations of the expansion at the third term yielding formulae (25),(26) and (27) for the radiation intensity, average energy and variance from which the STA spectrum is constructed as a Gaussian. The truncation of the Taylor expansion at the third term is justified in the short time limit. In the energy domain, it means a coarse graining of detailed structures finer than the variance of the STA. In contrast, in the CRSTA method, the summation to obtain  $\vartheta_{\Xi}^{ab}(\tau, \beta)$  is performed directly by the combinatorial steps (28)-(32), which yield the exact result in terms of a single CPPF (Eqs.(32) and in the general case equation (36),(37)). Out of the three assumptions, required for the derivation of the traditional STA method (*The basic superconfiguration assumption (a), the high-temperature approximation (b) and the unresolved supertransition array assumption (c)*), only the first one is used for the derivation of the CRSTA method. i.e. this new method utilizes the simplicity of the analytical manipulations, enabled by the basic superconfiguration assumption (a), without suffering from the spectral coarse graining imposed by the unresolved supertransition array assumption (c). This is the reason why in the numerical example, presented in figures (1)-(2), a detailed spectrum, which required half a million narrow STAs for its resolution, is resolved by a few CRSTAs.

The traditional STA concept was originally developed for plasmas at LTE. Later on, the idea was adapted also to the treatment of non-LTE plasma conditions (e.g. [32],[33]), and also to the treatment of the electronic degrees of freedom in the equation of state (e.g. [34]). The CRSTA method may be adapted also to these tasks.

The possibility to extend the method to resolutions beyond the UTA should also be explored. Another direction which should be explored is the incorporation of the CRSTA method with screened hydrogenic model (SHM e.g.[35]) into a code for rapid (possibly in-line) evaluation of opacity. The CRSTA method removes the calculational bottleneck of summation over transitions, while the SHM removes the calculational bottleneck of the SCF process and the evaluation of Slater integrals.

**Acknowledgement 1** *We thank N. Argaman for a carefull reading of the manuscript and many helpful remarks.*



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## VII. APPENDIX A: A FORMULA FOR THE SPECTRAL ABSORPTION COEFFICIENT ACCOUNTING FOR UTA WIDTH AND FIRST ORDER CORRECTION IN THE BOLTZMANN FACTOR.

The occupation numbers may be written as a vector of length of the number of shells,  $N_{\text{shell}}$ :

$$(\bar{q}^C)_r \equiv q_r^C.$$

Using this definition and the explicit form of the configurational average energy, center of gravity and variance of a UTA (Eqs.(13), (16) and (20) respectively), the scalar exponent  $\Phi_C^{ab}(\{q^C\}, \beta, \tau^2, i\tau)$  (Eq. (11)) may be written as a sum of three scalars; a scalar  $\Theta^{ab}$  which is independent of  $\bar{q}^C$ , a scalar product between  $\bar{q}^C$  and a vector of coefficients  $\vec{\Upsilon}^{ab}$  which is independent of  $\bar{q}^C$ , and a quadratic form in the vector  $\bar{q}^C$  with a real symmetric  $N_{\text{shell}} * N_{\text{shell}}$  matrix of coefficients,  $\overleftrightarrow{\Omega}^{ab}$ , which is independent of  $\bar{q}^C$ .

The quadratic form prevents a direct application of the combinatorial manipulations of Eqs (28)-(32). To cure this problem we diagonalize the matrix of coefficients,  $\overleftrightarrow{\Omega}^{ab}$ , and apply the Hubbard-Stratonovich transformation[24] (Eq. (34) below) which eliminates the nonlinear dependence on occupation numbers. Explicitly, this is done as follows:

First, the quadratic form is evaluated in a rotated system;

$$\vec{p}^C = \vec{q}^C \cdot \overleftrightarrow{R}^{ab},$$

which is chosen so that the matrix  $\overleftrightarrow{\Omega}^{ab}$  is diagonal. Explicitly, the elements of the  $k$  eigenvector of  $\overleftrightarrow{\Omega}^{ab}$  obey:

$$\sum_s \Omega_{rs}^{ab} R_{sk} = \lambda_k R_{rk}.$$

i.e.  $\overleftrightarrow{\Omega}^{ab}$  is diagonalized by a matrix with the elements  $R_{rk}$ ,

$$\begin{aligned} \left( \overleftrightarrow{\Lambda} \right)_{jk} &\equiv \sum_{s,r} R_{jr} \Omega_{rs} R_{sk} = \sum_r R_{jr} \lambda_k R_{rk} \\ &= \lambda_k \sum_r R_{jr} R_{rk} = \lambda_k \delta_{jk}, \end{aligned}$$

and  $\overleftrightarrow{\Omega}$  is obtained from  $\overleftrightarrow{\Lambda}$  by the inverse of this symmetric transformation:

$$\overleftrightarrow{\Omega} = \overleftrightarrow{R} \cdot \overleftrightarrow{\Lambda} \cdot \left( \overleftrightarrow{R} \right)^T.$$

Using Eq. (12) for the dipole matrix element together with the integral identity:

$$\exp \left( - \left( p_r^C \right)^2 \lambda_r^{ab} \right) = \sqrt{\frac{c_r}{2\pi}} \int_{-\infty}^{\infty} \exp \left( -\frac{1}{2} |c_r| x^2 + i x p_r^C \sqrt{2\lambda_r^{ab} |c_r|} \right) dx \quad (34)$$

the sum in Eq.(10) is written as:

$$\begin{aligned} U_{\Xi} \vartheta_{\Xi}^{ab} &= \\ &= \sum_{C \in \Xi} \left\{ f_C^{ab} g_C \exp \left\{ -\Theta - \sum_s q_s^C \Upsilon_s \right\} \right\} A_C^{ab} \end{aligned}$$

with

$$\begin{aligned} A_C^{ab} &= \prod_r \exp \left\{ - \left( p_r^C \right)^2 \lambda_r^{ab} \right\} \\ &= \prod_r \left\{ \sqrt{\frac{c_r}{2\pi}} \int_{-\infty}^{\infty} \exp \left( -\frac{1}{2} |c_r| x_r^2 + i x_r p_r^C \sqrt{2\lambda_r^{ab} |c_r|} \right) dx_r \right\} \\ &= \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \exp \left( -\frac{1}{2} \sum_r |c_r| x_r^2 + i \sum_s q_s^C \sum_r x_r R_{sr}^{ab} \sqrt{2\lambda_r^{ab} |c_r|} \right) \prod_r \sqrt{\frac{c_r}{2\pi}} dx_r \\ &= \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \exp \left( -\frac{1}{2} \sum_t \sum_s P_{st} \xi_s \xi_t + i \sum_s q_s^C \xi_s \right) \left| \left( \overleftrightarrow{T} \right)^{-1} \right| \prod_r \sqrt{\frac{c_r}{2\pi}} d\xi_r. \end{aligned} \quad (35)$$

The matrices  $\overleftrightarrow{T}$  and  $\overleftrightarrow{P}$  and the vector  $\vec{\xi}$  in Eq.(35) are defined by:

$$\left( \overleftrightarrow{T} \right)_{sr} = R_{sr}^{ab} \sqrt{2\lambda_r^{ab} |c_r|},$$

$$\left(\overleftarrow{P}\right)_{st} = \left(\sum_r c_r \left(\left(\overleftarrow{T}\right)^{-1}\right)_{rs} \left(\left(\overleftarrow{T}\right)^{-1}\right)_{rt}\right),$$

and:

$$\vec{\xi} = \overleftarrow{T} \cdot \vec{x}.$$

Next, define:

$$\Gamma^{ab}(\vec{\xi}) = \exp\left(-\frac{1}{2} \sum_t \sum_s P_{st} \xi_s \xi_t\right) \left| \left(\overleftarrow{T}\right)^{-1} \right| \prod_r \sqrt{\frac{c_r}{2\pi}}.$$

With this definition, the summation over configuration takes the form:

$$\begin{aligned} U_{\Xi} \vartheta_{\Xi}^{ab} &= \\ &= \sum_{C \in \Xi} \left\{ f_C^{ab} g_C \exp \left\{ -\Theta - \sum_s q_s^C \Upsilon_s \right\} \right\} A_C^{ab} \\ &= \sum_{C \in \Xi} \left\{ f_C^{ab} g_C \exp \left\{ -\Theta - \sum_s q_s^C \Upsilon_s \right\} \right\} \\ &\times \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \exp \left( -\frac{1}{2} \sum_t \sum_s P_{st} \xi_s \xi_t + i \sum_s q_s^C \xi_s \right) \left| \left(\overleftarrow{T}\right)^{-1} \right| \prod_r \sqrt{\frac{c_r}{2\pi}} d\xi_r \\ &= \exp \{ -\Theta \} (\langle a || r || b \rangle)^2 \\ &\times \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \left\{ \sum_{C \in \Xi} q_a^C (g_b - q_b^C) \prod_{s \in C} \binom{g_s}{q_s^C} [\exp \{ -(\Upsilon_s - i\xi_s) \}]^{q_s^C} \right\} \Gamma^{ab}(\vec{\xi}) d^{N_{\text{shell}}} \vec{\xi}. \end{aligned} \tag{36}$$

where the expression  $g_C = \prod_{s \in C} \binom{g_s}{q_s^C}$  for the configurational degeneracy was used.

Now define

$$\tilde{X}_s^{ab}(\beta, \tau) = \exp \{ -\Upsilon_s^{ab} + i\xi_s^{ab} \}$$

and the complex pseudo partition function:

$$\begin{aligned} \tilde{U}_Q^{ab} &\equiv \sum_{C \in \Xi} \prod_{s \in C} \binom{g_s}{q_s^C} \left( \tilde{X}_s^{ab} \right)^{q_s^C} \\ &= \sum_{C \{ \text{Sum}(q_s^C) = Q \}} \prod_{s \in C} \binom{g_s}{q_s^C} \left( \tilde{X}_s^{ab} \right)^{q_s^C}, \end{aligned} \tag{37}$$

and apply the same combinatorial steps as in Eq.(32). The result is a the generalization of Eq. (33):

$$\begin{aligned}
\mu_{\text{at}}(E) &= \frac{4\pi}{3} \frac{e^2}{\hbar c} \frac{E}{\hbar} n_0 (1 - e^{-\beta E}) \frac{1}{U|_{\tau=0}} \sum_{\Xi, a, b} (\langle a || r || b \rangle)^2 g_a g_b \\
&\times \text{Re} \int_0^\infty d\tau \left\{ \exp \{ -\Theta^{ab}(\tau) \} \int_{-\infty}^\infty d^N \vec{\xi} \left\{ \tilde{X}_a^{ab}(\vec{\xi}) \tilde{U}_{\Xi, Q-1}^{ab}(\vec{g} - \vec{\delta}_a - \vec{\delta}_b, \beta, \tau, \vec{\xi}) \Gamma^{ab}(\vec{\xi}) \right\} \right\}.
\end{aligned} \tag{38}$$

Eq.(38) is a formula for the spectral absorption coefficient which accounts for the width of the UTA, as well as the first order correction in the Boltzmann factor without the restriction of the high temperature approximation.